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This document lists the problems that we encountered in processing ENDF/B-VI.r8 that we suspect are problems with ENDF/B-VI.r8 itself. It also contains a comparison of linear interpolation methods. Finally, this document proposes an alternative to the current scheme of reporting problems to the ENDF community.

We have found several problems with the latest release of ENDF/B-VI. Many of these problems are small and a few are large. In this document, we list the problems that we found, we comment on the problems with various linear interpolation schemes and we comment on a possible scheme to streamline the bug reporting for ENDF/B-VI.

I. DATABASE BUGS

The data base bugs are organized by nuclide or by topic (such as the discussion of interpolation type 12).

A. Deuterium (MAT=128)

There is an error in ENDF/B-VI tape 137 at line 646. The offending line is show in Fig. 1. The section refers to the outgoing proton from the d(n,2n)p reaction, so the first column should be 1.001000+3.

B. ^{14}N (MAT=725)

There is a problem with the ^{14}N (MAT=725) evaluation in ENDF/B-VI. There are gamma production files (MF=13 and 14) for reactions MT=28 and MT=32 but no cross section files for these reactions or other outgoing particle information. Either the gamma data should be deleted or the missing information added in the next update.

C. ^{209}Bi (MAT=8325)

It appears as though there is an error in the ENDF/B-VI data for ^{209}Bi. In the first line of the MF=4 MT=2 section, LTT is set to 3, as seen in Fig. 2 Since the data is a table of Legendre coefficients, LTT should be set to 1.

D. ^{233}Pa (MAT=9137)

In the MF=5, MT=9 entry, (corresponding to inelastic scattering to the continuum, (z,n$_c$)), there are two 2.000000+5 incident neutron energies with different Θ's (1.000000+4 and 9.430710+4) in a linear interpolation table. The entire entry is reproduced in Fig. 3. Taken at face value, the entry says to interpolate from 2.000000+5 to 2.000000+5, so the first 2.000000+5 gets ignored. This seems odd and we wonder if maybe only one of the 2.000000+5 pairs is supposed to be used. If so, then which one?

E. ^{233}U (MAT=9222)

[ENDF/B-VII beta update is available, but we have not checked it]

In the ^{233}U evaluation, both MT=3 and MT=4 are used for the gammas. MT=3 is supposed to be a sum of MT=4,5,11,16-18,22-26,28-37,41-42,44-45,102-117. However, it is clear that this is not the case in this evaluation. Instead, one MT is used for energies below 1.09 MeV and the other above.

F. ^{237}Np (MAT=9346)

[ENDF/B-VII beta update is available, but we have not checked it]

There are two problems with this evaluation: a typo and two conflicting options. The typo in the ENDF/B-VI file involves a permutation of 2 digits in line 16340 (MF=12 data for MT=59). The third entry in the line is 5.935700+4, and it ought to be 5.953700+4. What happens here is that the MF=12 file gives the probability of jumping to various levels, and we are trying to jump to a level which does not exist.

The other problem is that discrete gamma data for inelastic (n, n') is represented as a continuum cascade with the gamma energy shifted by a mass ratio. This is the result of a mix of 2 incompatible ENDF/B-VI options:

- For inelastic scattering the evaluator may represent the data as energy levels with branching ratios for the jumps to the lower levels (LO=2).
- For compound reactions the continuum gammas may be represented as a set of discrete lines (LO=1), and there is a rule for shifting the frequencies of these lines, depending on the energy of the incident particle (LP=2).

```
1.001000+0 9.986200-1          0          6          1          2 128 6 16  646
```

FIG. 1: Offending line in deuterium evaluation.

```
8.320900+4 2.071850+2          0          3          0 08325 4  2    1
```

FIG. 2: Offending line in ^{209}Bi evaluation.

It makes no sense say that the discrete lines from inelastic scattering (MT = 51, 52, ..., MT < 91) represent a gamma continuum, but that is what is in the ENDF/B-VI file. (The flag is set LO = 2 in place of LO = 1.)

G. ^{249}Bk (MAT=9752)

There are two identical copies of an outgoing neutron outgoing distribution for $E_{in} = 6.5$ MeV in the first (n,n') reaction (MT=51,MF=4).

H. Interpolation Type 12

We do not understand the documentation for interpolation type 12, also known as the Method of Corresponding Points. The definition given in Ref. [4] allows for the situation pictured in Fig. 4. In this figure, the number of energies in the interpolation table undergoes a jump from 2 points to 3 (in practice, the jump can go from 2 points to 4!).

The question for us is what to do in the region between points A, B, and C. A naive interpretation of the documentation would suggest that we treat this as just a step in energy. We would have to renormalize probability distributions going across the step in some (as yet unspecified) way. Another possibility is to do some form of "triangular" interpolation to go from point A to point C.

We have found this problem is several reactions, including some in the evaluations for ^{25}Mn and ^{28}Ni.

II. INTERPOLATION COMMENTS

In this section, we present some concerns regarding the writeup on unit-base interpolation in ENDF/B-VI.

We consider a very simple case in this note to make things as clear as possible. In this example, all energies are dimensionless. If we understand this case, then the extension to the general case is straightforward.

Suppose that for energy of the incident neutron $E = 0$ we have 2 data points $(E'p)$ for the energy distribution, one at $E' = 0$ and one at $E' = 1$. We use linear interpolation for the probability density p at intermediate energies of the emitted particle, $0 < E' < 1$. Similarly, for incident neutron energy $E = 1$ suppose that we have 2 data points, one at $E' = 0$ and one at $E' = 1+\beta$. (This is interesting only if $\beta \neq 0$.) Again, for $E = 1$ we use linear interpolation with respect to E' for $0 < E' < 1+\beta$. The situation is illustrated in Fig. 5

The question is how to do the interpolation with respect to the incident energy E. We want this interpolation to ensure proper normalization of the probability density. That is, we want to have

$$I(E) = \int_0^{1+\beta E} p(E, E')\, dE' = 1$$

for every value of E in $0 \leq E \leq 1$, assuming that the original data at $E = 0$ and $E = 1$ is so normalized. In this note I describe 3 "reasonable" interpolation methods and show that only the traditional ENDL method gives proper normalization.

A. Simple bilinear interpolation.

The interpolation scheme that once seemed most natural to me is bilinear interpolation

$$p(E, E') = \alpha_0 + \alpha_1 E + \alpha_2 E' + \alpha_3 E E'.$$

The coefficients α_j are determined by requiring that $p(E, E')$ take on the given values at the 4 original data points.

To show that this interpolation scheme violates the normalization, it is sufficient to observe that integration of this function over $0 \leq E' \leq 1 + \beta E$ gives a cubic polynomial in E and that the coefficient of E^3 in this cubic is $\alpha_3\beta^2/2$. In general this coefficient is not zero, so we really do have a cubic. Its value is 1 at $E = 0$ and at $E = 1$, but it can't be 1 for all intermediate values of E.

B. ENDF-style unit-base interpolation

The version of unit-base interpolation given on the ENDF manual [4] is as follows. We first do a mapping

$$E = \xi, \qquad E' = (1 + \beta\xi)\eta,$$

with $0 \leq \xi \leq 1$ and $0 \leq \eta \leq 1$. In these coordinates the normalizaton condition takes the form

$$\int_0^1 p \frac{\partial E'}{\partial \eta}\, d\eta = 1$$

```
9.123300+4 2.310380+2          0          0          1          09137 5 91  944
1.878100+4 0.000000+0          0          9          1          29137 5 91  945
         2          2                                                9137 5 91  946
2.000000+5 1.000000+0 2.000000+7 1.000000+0                          9137 5 91  947
0.000000+0 0.000000+0          0          0          2          49137 5 91  948
         2          2          4          5                     9137 5 91  949
2.000000+5 1.000000+4 2.000000+5 9.430710+4 1.500000+7 8.167240+59137 5 91  950
2.000000+7 9.430720+5                                                9137 5 91  951
```

FIG. 3: Offending lines in ^{233}Pa evaluation.

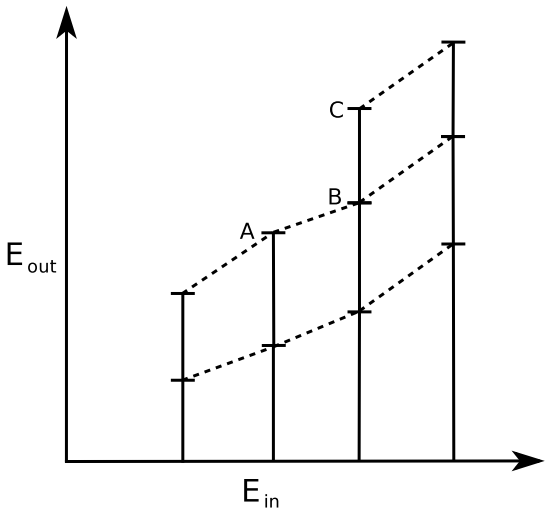

FIG. 4: Cartoon illustrating the confusion with interpolation type 12, the Method of Corresponding Points.

The suggestion is to do bilinear interpolation of p as

$$p = \alpha_0 + \alpha_1\xi + \alpha_2\eta + \alpha_3\xi\eta.$$

We are to multiply this function by

$$\frac{\partial E'}{\partial \eta} = (1 + \beta\xi)$$

But the integral of this product over $0 \leq \eta \leq 1$ is a quadratic in ξ. Except when $\beta = 0$, this quadratic takes the value 1 only at the points $\xi = 0$ and $\xi = 1$. So, this interpolation scheme doesn't work either.

C. ENDL-style unit-base interpolation

The method of unit-base interpolation given in the Omega manual [5] differs from that in the previous paragraph only in that we renormalize the probability density before doing the bilinear interpolation. Specifically, we use

$$p\frac{\partial E'}{\partial \eta} = \alpha_0 + \alpha_1\xi + \alpha_2\eta + \alpha_3\xi\eta.$$

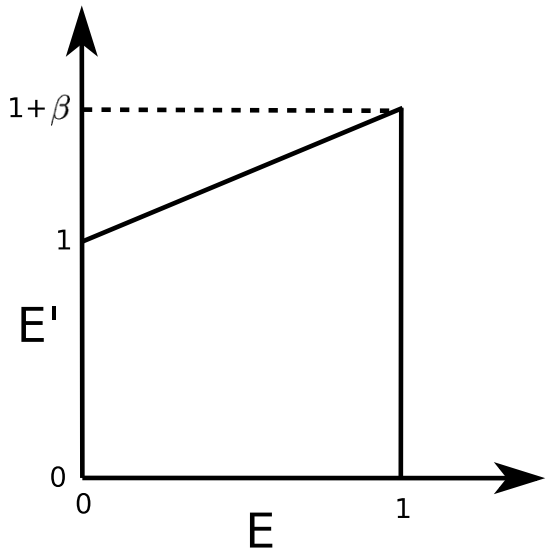

FIG. 5: Linear interpolation example. The text describes three separate schemes for interpolating in this case.

The integral of this function over $0 \leq \eta \leq 1$ is a linear function of ξ. It takes the value 1 at $\xi = 0$ and $\xi = 1$, so its value is 1 for all ξ between 0 and 1.

We would prefer to do ENDL-style unit-base interpolation on each segment of the type-12 pairwise-points scheme, rather than the scheme detailed above.

III. THOUGHTS ON AUTOMATED BUG REPORTING

We believe that most (if not all) of these problems have been discovered by others and it is possible that some of these have already been fixed. Thus, there is possibly a large duplication of effort in the compilation of this

list. The recent posting of the "buglist" on the CSEWG member page [1] is a huge step toward eliminating future duplication of effort, but maintaining this page requires a an investment in manpower. We advocate moving to an automated web-based bug tracking system. Moving to such a system has several advantages over the current system:

- One can immediately see if your problem is caused by one's own bug or is a database bug.
- One can see if a known bug is fixed/in progress of being fixed.
- One can post a bug so others don't have to stumble across it themselves.
- Provides an open record of bugs found and killed.
- ENDFB-VI is an open, international, effort; currently our bug reporting is only partly so.

One such tool is `bugzilla` [2], but surely others exists too. This suggestion not meant as a replacement for the peer review process. `bugzilla` or equivalent would supplement the current process in much the same way that preprint servers supplement peer reviewed journals.

Acknowledgments

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[1] V. McLane, "Known Errors and Deficiencies in ENDF/B-VI," `http://www.nndc.bnl.gov/csewg_members/errors.html`.
[2] `bugzilla` Project Homepage, `http://www.bugzilla.org/`.
[3] Evaluated Nuclear Data File, `http://www.nndc.bnl.gov/nndc/endf/`.
[4] Cross Section Evaluation Working Group, "ENDF-102 Data Formats and Procedures for the Evaluated Nuclear Data File ENDF-6," Ed. V. McLane, C.L. Dunford, P.F. Rose, Brookhaven National Laboratory Report BNL-NCS-44945, (1997).
[5] R. J. Howerton, R. E. Dye, P. C. Giles, J. R. Kimlinger, S. T.Perkins, and E. F. Plechaty, "Omega: A Cray 1 executive code for LLNL nuclear data libraries", Lawrence Livermore National Laboratory Report UCRL-50400, Vol. 25 (1983).